Intrinsic-Density Functionals

J. Engel*

Department of Physics and Astronomy, CB3255,
University of North Carolina, Chapel Hill, NC 27599-3255

(Dated: October 10, 2006)

Abstract

The Hohenberg-Kohn theorem and Kohn-Sham procedure are extended to functionals of the localized intrinsic density of a self-bound system such as a nucleus. After defining the intrinsic-density functional, we modify the usual Kohn-Sham procedure slightly to evaluate the mean-field approximation to the functional, and carefully describe the construction of the leading corrections for a system of fermions in one dimension with a spin-degeneracy equal to the number of particles N. Despite the fact that the corrections are complicated and nonlocal, we are able to construct a local Skyrme-like intrinsic-density functional that, while different from the exact functional, shares with it a minimum value equal to the exact ground-state energy at the exact ground-state intrinsic density, to next-to-leading order in $1/N$. We briefly discuss implications for real Skyrme functionals.

*engelj@physics.unc.edu

I. INTRODUCTION

The Hohenberg-Kohn theorem [1] and the associated Kohn-Sham procedure [2] have helped to shift the interpretation of Skyrme-mean-field theory in heavy nuclei. Nowadays, instead of focusing on a Skyrme nucleon-nucleon interaction, theorists start with a Skyrme (or relativistic) mean-field-like density functional, modifying its parameters to fit nuclear properties in ways that are not obviously consistent with the existence of an underlying effective two-body interaction. The Hohenberg-Kohn theorem is often used to justify this step, the idea being that Skyrme functionals are an approximation to a universal Kohn-Sham density functional — written in terms of single-particle orbits and leading to Hartree-like equations — that is guaranteed to include all correlations.

Because the nucleus is a self-bound system, however, the usual Hohenberg-Kohn theorem is not really a justification. It states that there exists a universal functional of a system's *laboratory* density that has a minimum at the ground state density, and that the value of the functional at the minimum is the ground-state energy. The adjective "universal" means that the functional can be written as a sum of a part that is independent of whatever external one-body potential the system is in — the universal part — and a simple term $\int V(\boldsymbol{r})\rho(\boldsymbol{r})d\boldsymbol{r}$, where V is the one-body potential and ρ is the usual laboratory density. The density of interest in nuclear physics, however, is the *intrinsic* density, i.e. the density relative to the nuclear center of mass, not relative to a fixed point in the lab. It is this intrinsic density that is localized and measured in scattering experiments. By contrast, the laboratory nuclear density of an isolated nucleus is spread out evenly over all space because the nuclear center of mass is free to move anywhere. Thus, the universal Hohenberg-Kohn functional has a minimum at a constant spread-out density that contains no information about the localized intrinsic density. The guaranteed existence of this functional is irrelevant to nuclear physics. The same is true of the usual Kohn-Sham procedure, which represents the density as a sum of squares of single-particle wave functions, leading to a Hartree-like equations for the ground-state density and energy. The single-particle orbitals for the ground-state laboratory density are plane waves.

Because the ground state wave function of the nucleus factors into center-of-mass and intrinsic parts, it is possible — by removing the center-of-mass kinetic energy from the Hamiltonian and adding a potential such as $V_{CM} \equiv (\sum_i \boldsymbol{r}_i)^2$ that is minimized when the center of mass is at the origin — to construct a related Hamiltonian for which the ground-state laboratory density is the same as the intrinsic density. One could then try to produce an ordinary density functional for this new Hamiltonian, assured by the Hohenberg-Kohn theorem that its minimum would yield the true intrinsic density. By making the potential very weak, one could even make the functional yield the true ground-state energy when minimized. This procedure, however, would single out one point in space and would therefore look very different from Skyrme mean-field theory, in which the functional is minimized by a family of Slater determinants, related to one another by translation. Furthermore, the local-density approximation (LDA) and extensions, through which Skyrme functionals might be derived [3], could easily destroy the conditions that force the intrinsic density to be the same as the laboratory density. The whole Skyrme enterprise would make much more sense if we knew that we could construct an exact Kohn-Sham functional of of the intrinsic density rather than the laboratory density, without modifying the Hamiltonian.

These considerations, and related ones connected with deformation and rotation, lead us to ask whether analogs of the Hohenberg-Kohn theorem and Kohn-Sham procedure exist

for the intrinsic density. Rotation is more complicated than translation because it doesn't decouple from internal motion and because the intrinsic rotational density is not directly observable, so for now we worry only about translation and define the intrinsic density simply as the density with respect to the center of mass. The operator corresponding to that quantity is

$$\hat{\rho}_I(\boldsymbol{r}) \equiv \hat{\rho}(\boldsymbol{r} + \hat{\boldsymbol{r}}_{\rm CM}) \ , \tag{1}$$

where $\hat{\rho}$ is the usual laboratory density operator, the center-of-mass position operator $\hat{r}_{\rm CM}$ is defined by

$$\hat{\boldsymbol{r}}_{\rm CM} \equiv \frac{1}{N} \sum_{i=1}^{N} \hat{\boldsymbol{r}}_i \ , \tag{2}$$

and the hats over ρ_I, ρ, $\boldsymbol{r}_i$, and $\boldsymbol{r}_{\rm CM}$ are to emphasize that the quantities are operators, unlike the variable $\boldsymbol{r}$ in Eq. (1). The intrinsic density, unlike its lab-frame counterpart, is an N-body operator, complicating density-functional theory for self-bound systems.

In the next section we address the question of whether there is an analog of the Hohenberg-Kohn theorem guaranteeing the existence of an intrinsic "universal" intrinsic-density functional with a minimum at the exact ground-state intrinsic density and energy. Section III argues that a Kohn-Sham-like procedure can be used to find the exact intrinsic density, and outlines the construction of the corresponding Kohn-Sham equations. We will work with a specific one-dimensional model to simplify the formalism, but will carry the construction as far as possible; as a result this section is the longest and most technical. In section IV we produce a phenomenological Skyrme-like functional that, while not exact away from the minimum, does yield the model's exact intrinsic density and energy at its minimum to good accuracy. We then briefly discuss the implications of these results for real three-dimensional nuclear physics.

II. HOHENBERG-KOHN THEOREM FOR INTRINSIC DENSITY

There is indeed a Hohenberg-Kohn theorem for the intrinsic density. In fact, Valiev and Fernando [4] have shown — assuming a nonrelativistic Hamiltonian, and using an effective-action formalism invented in Ref. [5] — that given *any* Hermitian operator $\hat{Q}(\boldsymbol{r})$, one can construct an energy functional $E[Q]$ that is universal in a sense to be discussed and has a unique (and correct) minimum at $Q(\boldsymbol{r}) = \langle \hat{Q}(\boldsymbol{r}) \rangle_{\rm gs}$, the ground-state expectation value of $\hat{Q}(\boldsymbol{r})$. Introducing a "source" $J(\boldsymbol{r})$ that couples to $Q(\boldsymbol{r})$ and alters the ground-state energy:

$$\mathcal{E}[J] \equiv \langle \hat{H} + \int J(\boldsymbol{r}) \hat{Q}(\boldsymbol{r}) d\boldsymbol{r} \rangle_{\rm gs}^{J} \ , \tag{3}$$

one can define the functional $E[Q]$ as the functional Legendre transform with respect to J. In other words

$$E[Q] = \mathcal{E}[J[Q]] - J[Q] \circ Q \quad , \tag{4}$$

where $J[Q](\boldsymbol{r})$ is the particular source function that makes $\langle \hat{Q}(\boldsymbol{r}) \rangle_{\rm gs}^{J} = Q(\boldsymbol{r})$, and we have used the convention $A \circ B \equiv \int A(\boldsymbol{r}) B(\boldsymbol{r}) d\boldsymbol{r}$. It's not hard to show [6] (and this is an alternative and perhaps clearer definition) that $E[Q]$ is the minimum of $\langle \hat{H} \rangle$ over all normalized N-particle wave functions that have $\langle \hat{Q}(\boldsymbol{r}) \rangle = Q(\boldsymbol{r})$. Since $\langle \hat{H} \rangle$ is smallest in the ground

state, the functional is minimized when $Q \equiv \langle \hat{Q} \rangle_{\rm gs}$. It is universal in that the addition of an arbitrary term $V \circ \hat{Q}$ to the Hamiltonian merely adds $V \circ Q$ to $E[Q]$.

All this means, in particular, that for nuclei there is a universal "intrinsic-density functional" $E[\rho_I]$ with a minimum at the ground-state intrinsic density, and that we know in principal how to construct it. It's worth noting that the functional is not universal under the addition of an ordinary one-body potential $\sum_i V(\hat{\boldsymbol{r}}_i)$ to the Hamiltonian, but rather the addition of a generically N-body potential $\sum_i V(\hat{\boldsymbol{r}}_i - \hat{\boldsymbol{r}}_{\rm CM})$ that affects only intrinsic structure.

The important question, though, is how to incorporate orbitals into this framework in a way that leads to a constructive procedure for the energy functional. In other words, can one derive a Kohn-Sham-like (e.g. Skyrme-like) functional for the intrinsic density, even in principle? In the next section we show that one can.

III. ORBITALS AND KOHN-SHAM-LIKE EQUATIONS

A. Framework

Refs. [4, 7] introduce Kohn-Sham orbitals in functionals of the ordinary density (in systems that are not self bound) through the perturbative "inversion method" [8]. In this approach one divides $\tilde{J}[\rho]$, where the tilde here and below distinguishes the quantity from the related one to be used here for the intrinsic density ρ_I, into a piece $\tilde{J}_0[\rho]$, the Kohn-Sham potential that forces a *noninteracting* system to have the density ρ, and the rest. The entire functional can be constructed from $\tilde{J}_0$ and expressed in terms of the noninteracting orbitals ϕ_k and energies ϵ_k that $\tilde{J}_0$ determines. In our notation, under the assumption that $\tilde{\mathcal{E}}[\tilde{J}]$ can be divided into successively smaller contributions $\tilde{\mathcal{E}}[\tilde{J}] = \tilde{\mathcal{E}}_0[\tilde{J}] + \tilde{\mathcal{E}}_1[\tilde{J}] + \cdots$, the energy-density functional $\tilde{E}[\rho]$, has the form [4, 7]

$$\tilde{E}[\rho] = \tilde{E}_0[\rho] + \tilde{E}_{\rm int}[\rho] \ , \tag{5}$$

where

$$\tilde{E}_0[\rho] = \tilde{\mathcal{E}}_0[\tilde{J}_0] - \tilde{J}_0 \circ \rho \ , \qquad \tilde{E}_{\rm int}[\rho] = \tilde{\mathcal{E}}_1[\tilde{J}_0] + \cdots \ , \tag{6}$$

and we have truncated $\tilde{E}_{\rm int}[\rho]$ at lowest order. To find the ground-state density and energy one rewrites the minimization condition $\delta\tilde{E}[\rho]/\delta\rho = 0$, as an implicit Kohn-Sham equation of the form

$$\frac{\delta \tilde{E}_{\rm int}[\rho]}{\delta\rho} = \tilde{J}_0[\rho] \ , \tag{7}$$

where we have used Eq. (5) and the fact that $\delta\tilde{E}_0/\delta[\rho] = -\tilde{J}_0$, which follows from the definition of $\tilde{E}_0$ as a Legendre transform. The Kohn-Sham procedure then consists of choosing a trial potential $\tilde{J}_0$, solving the single-particle Schroedinger equation to obtain the corresponding ϕ_k and ϵ_k, computing $\tilde{E}_{\rm int}$ and $\delta\tilde{E}_{\rm int}/\delta\rho$ in terms of these quantities, and then iterating until the energy and density converge. The procedure amounts to solving Hartree equations with the mean-field potential $V[\rho] = \delta\tilde{E}_{\rm int}/\delta\rho$.

We can apply this procedure to our intrinsic functional $E[\rho_I]$, even though ρ_I is an N-body operator, provided we start at a slightly different point: mean-field theory. To make the discussion less abstract, we refer explicitly to a simple one-dimensional system. Before constructing an energy functional, we describe the system, its exact ground-state energy and intrinsic density, and the mean-field approximations to these quantities.

B. Model in one dimension

We consider N fermions with spin-degeneracy N interacting via an attractive two-body delta function ($\hbar = 1$):

$$H = -\frac{1}{2m}\sum_{i=1}^{N}\frac{d^2}{dx_i^2} - g\sum_{i<j}\delta(x_i - x_j) \quad . \tag{8}$$

This model has the nice feature of being exactly solvable. The ground state is bound and the corresponding energy and intrinsic density are known [9, 10]:

$$E_{\rm gs} = \frac{1}{24}mg^2(N^3 - N) \tag{9}$$

$$\rho_I^{\rm gs}(x) = mg\sum_{n=1}^{N-1}(-)^{n+1}\frac{n(N!)^2 e^{-nNmg|x|}}{(N+n-1)!(N-n-1)!} \tag{10}$$

$$= \frac{mgN^2}{4{\rm cosh}^2(\frac{Nmgx}{2})}\left(1 - \frac{1}{N}\left[1 - \frac{3}{2{\rm cosh}^2(\frac{Nmgx}{2})}\right] + \mathcal{O}(\frac{1}{N^2})\right) \ , \qquad mg|x| \gtrsim \frac{3\,{\rm ln}N}{N^2} \ .$$

The ground state differs from that of a nucleus, however, in that the system shrinks to a point as N increases and the binding energy goes like N^3; there is nothing resembling saturation. A local-density approximation for such a system, which has no uniform limit, is hard to imagine.

Ref. [10] analyzed the Hartree-Fock approximation, to which we refer as the mean-field approximation, for the ground state. The approximation is improved when the center-of-mass kinetic energy is subtracted from the Hamiltonian, as e.g. in the no-core shell model [11]. Subtraction makes a localized ground-state possible, since the center-of-mass is no longer required to be in a plane-wave state. Because the spin degeneracy is equal to the number of particles, whether or not one subtracts, the spatial mean-field orbital $\phi(x)$ is the same for every particle. The mean-field equation for ϕ, with no external source and the center-of-mass kinetic energy subtracted, is

$$-\frac{N-1}{2mN}\phi''(x) - (N-1)g|\phi(x)|^2\phi(x) = \epsilon\phi(x) \tag{11}$$

Because of translational invariance, the solutions make up a degenerate set with each member centered at a different point $x = a$ in space:

$$\phi(x) = \frac{\sqrt{Nmg}}{2{\rm cosh}[Nmg(x-a)/2]} \ , \qquad \epsilon = -\frac{mg^2}{8}N(N-1) \ . \tag{12}$$

The average position $\bar{x}$, given by

$$\bar{x} = \int x|\phi(x)|^2 dx \ , \tag{13}$$

is just $\bar{x} = a$ for the mean-field solutions. The mean-field energy is then

$$\begin{aligned} E_{\rm mf} &= N(N-1)\int dx \left[\frac{1}{2mN}|\phi'(x)|^2 - \frac{g}{2}|\phi(x)|^4\right] \\ &= N\epsilon + \frac{N(N-1)g}{2}\int |\phi(x)|^4 dx \\ &= -\frac{mg^2}{24}N^2(N-1) \end{aligned} \tag{14}$$

Interestingly, the mean-field energy is correct at leading order in the small quantity $1/N$, that is, the $\mathcal{O}(N^3)$ term is right. At $\mathcal{O}(N^2)$ there is an error; the exact energy in Eq. (9)has no term of that order. The mean-field $\mathcal{O}(N^2)$ energy is reduced by the subtraction of the center-of-mass kinetic energy, but, as Ref. [12] shows, one needs to include ring diagrams[1] (i.e. the RPA correlation energy) to cancel it completely.

The mean-field laboratory density $N\phi^2(x)$ is also correct in some sense in leading order; because center-of-mass motion becomes irrelevant at large N, the mean-field laboratory density reproduces the exact intrinsic density there, assuming the center of mass is at the origin [10]. The mean-field *intrinsic* density can be computed by expanding the operator $\hat{\rho}_I(x) \equiv \hat{\rho}(x + \bar{x} + \hat{x}_{\rm CM} - \bar{x})$ around $x + \bar{x}$ in powers of $\hat{x}_{\rm CM} - \bar{x}$, leading, after some algebra, to

$$\begin{aligned} \langle\hat{\rho}_I(x)\rangle_{\rm mf} &= c_N N\left[|\phi(c_N x + \bar{x})|^2 + \frac{\mu}{2N}\frac{d^2}{dx^2}|\phi(c_N x + \bar{x})|^2 + \mathcal{O}(\frac{1}{N^2})\right] \\ &= N\left[|\phi(x+\bar{x})|^2 + \frac{1}{N}\left(|\phi(x+\bar{x})|^2 + x\frac{d}{dx}|\phi(x+\bar{x})|^2 + \frac{\mu}{2}\frac{d^2}{dx^2}|\phi(x+\bar{x})|^2\right) + \mathcal{O}(\frac{1}{N^2})\right] , \end{aligned} \tag{15}$$

with

$$\mu = \int (x-\bar{x})^2|\phi(x)|^2 dx \quad , \qquad c_N = \frac{N}{N-1} \tag{16}$$

Beyond leading order, this expression gives a better approximation to the exact intrinsic density than does the mean-field laboratory density $N|\phi(x)|^2$, as can be seen, for example, by using it to compute the $\langle x^2\rangle_{\rm intr}$. The result, $\langle x^2\rangle_{\rm intr} = \mu(1 - \frac{1}{N})$, is the same as the exact one.

With these results in hand, we can move to the construction of a Kohn-Sham-like intrinsic-density functional for the model.

C. Intrinsic Density Functional at Mean-Field Level

The problem with applying the Kohn-Sham procedure directly to the intrinsic density is that the source term, $J_0 \circ \hat{\rho}_I$, is an N-body operator. We cannot treat the source exactly and still have a noninteracting system, the starting point for the inversion method discussed

[1] One might mistakenly infer from Ref. [12] that ring diagrams with more than two rings contribute very little to the $\mathcal{O}(N^2)$ correlation energy. That can appear to be so, but only if one modifies the Hamiltonian (by subtracting the center-of-mass energy) in the Hartree-Fock calculation but neglects to do so in the RPA.

above. Instead, we start with the mean-field approximation, not just for the true ground-state, but also for the ground state with the addition of the term $J_0 \circ \hat{\rho}_I$. In other words, $J_0[\rho_I]$ is now the source function that forces the intrinsic density to be ρ_I when the system is treated in *mean-field approximation*. The resulting mean-field single-particle orbitals will play the same role in obtaining the exact intrinsic functional as Kohn-Sham orbitals for a noninteracting system do in the usual approach, and the inversion method will go through without any other modifications. Of course, to apply it we must assume that corrections to mean-field theory are perturbative. For the model just described that is certainly the case, as we shall see. For real Skyrme functionals, it is not unreasonable to assume the existence of an effective Hamiltonian for which Hartree-Fock is a good starting point, at least in spherical nuclei.

Constructing the mean-field intrinsic-density *functional* as the first term $E_0[\rho_I]$ in the intrinsic version of Eq. (5) can be done without solving any equations. We are supposed to start with

$$\mathcal{E}_0[J_0] = N(N-1)\int dx \left[\frac{1}{2mN}|\phi'(x)|^2 - \frac{g}{2}|\phi(x)|^4\right] + J_0 \circ \langle\hat{\rho}_I\rangle_{\rm mf} \ , \tag{17}$$

where $\langle\hat{\rho}_I\rangle_{\rm mf}$ is given by Eq. (15) and we have taken the useful but not essential step of subtracting the center-of-mass kinetic energy (though without explicitly writing a more complicated two-body center-of-mass term that has no effect on bound states) to improve the mean-field approximation. But since J_0 is supposed to be fixed so that $\langle\hat{\rho}_I\rangle_{\rm mf} = \rho_I$ and then $J_0 \circ \rho_I$ subtracted from $\mathcal{E}_0[J_0]$, the mean-field functional looks just like the first line of Eq. (14):

$$E_0[\rho_I] = N(N-1)\int dx \left[\frac{1}{2mN}|\phi'(x)|^2 - \frac{g}{2}|\phi(x)|^4\right] \tag{18}$$

This simple Skyrme-like object, when written in terms of the orbital ϕ, is the same as the mean-field functional one would get for the ordinary one-body density, but now ϕ *is a functional of* ρ_I (up to the location of the center of mass $\bar{x}$, which must also be specified) rather than ρ. The relation between the two functionals is not surprising because at mean-field level the Slater determinant constructed from orbital ϕ is the system's wave function, and the energy functional — the energy corresponding to that wave function — is just the expectation value of the Hamiltonian, no matter what observable we write the functional (and ϕ) in terms of. (When we go beyond mean-field theory, center-of-mass motion makes the functionals of the lab and intrinsic density quite different.)

In more detail, ϕ is a functional of ρ_I in the following sense: ρ_I determines J_0 through the solution to $\delta\mathcal{E}_0/\delta J_0 = \rho_I$ (Ref. [4] shows that the solution exists and is unique) and J_0 determines ϕ, again up to its overall location, through the solution to the mean-field equations, which we haven't yet written, that come from varying $\mathcal{E}_0[J_0]$ with respect to ϕ (with a constraint on its norm). With ϕ and E_0 functionals of ρ_I, one can then reproduce the mean-field ground-state energy and intrinsic density by solving the equation $\delta E_0/\delta\rho_I = 0$. Because this equation says that $J_0 = 0$, finding the minimum corresponds to solving the source-free mean-field equation, *i.e.* the Hartree equation Eq. (11), and then computing ρ_I from Eq. (15). This Hartree equation is the leading approximation to the Kohn-Sham-like equation we seek.

All this may seem pedantic, but it contains an important point about the relation of ϕ to ρ_I: the condition $\delta\mathcal{E}_0/\delta J_0 = \rho_I$ simply states that ρ_I will be given in terms of ϕ by Eq. (15), with ρ_I replacing $\langle\hat{\rho}_I\rangle_{\rm mf}$. Thus, though $\rho_I(x)$ is just $N|\phi(x+\bar{x})|^2$ to leading order in $1/N$, it

has higher-order corrections. This fact is apparently important for real Skyrme functionals, which fit data best when a prescription [13] for ρ_I that approximates the real-world analog of the Eq. (15) is used to calculate observables such as the rms radius [14]. Using the uncorrected expression $\rho_I(x) \equiv \sum_k |\phi_k(x+\bar{x})|^2$ for this purpose produces noticeably poorer results.

It actually is possible to formulate an intrinsic-density functional theory in which $\rho_I \equiv \sum_k |\phi_k(x+\bar{x})|^2$ without corrections. In the simple model we can do so by neglecting the $\mathcal{O}(1/N)$ terms in Eq. (15) when defining $\mathcal{E}_0[J_0]$, and taking their effects into account at the next level of approximation. Such a step would in fact simplify much of the formalism to come, e.g., the mean-field equation for the orbital ϕ in the presence of the many-body source J_0. And when expressing the leading-order intrinsic-density functional in terms of ϕ we'd still end up with Eq. (18). That object, however, would be a different functional of ρ_I than before and would produce poorer results for the ground-state intrinsic density. We will not elaborate the corrections to the functional necessary to restore the lost accuracy, lest this paper get even longer than it is. Instead, using the relation between ρ_I and ϕ given by Eq. (15), we proceed to take up corrections that are genuinely beyond mean-field theory. Though the lack of something like the LDA prevents us from actually calculating the corrections, either analytically or numerically, we describe how to do the latter, in some detail.

D. Beyond Mean-Field Theory

To go beyond the relatively straightforward mean-field approximation to $E[\rho_I]$, one would need to calculate $E_{\rm int}[\rho_I] = E_1[\rho_I] + \cdots = \mathcal{E}_1[J_0] + \ldots$. (We content ourselves with E_1 here, though we could go further.) Then, provided one could calculate $\delta E_1/\delta\rho_I(x)$, one could follow the procedure Kohn-Sham procedure outlined above, rewriting the minimization condition $\delta E[\rho_I]/\delta\rho_I$ in the form

$$J_0(x) = \frac{\delta\mathcal{E}_1[J_0]}{\delta\rho_I(x)} \ . \tag{19}$$

and solving by iteration, starting with a guess for J_0. We will call Eq. (19) the Kohn-Sham equation, even though strictly speaking it doesn't involve Kohn-Sham orbitals.

Given a J_0, one could find $\mathcal{E}_1$ in the following way: The first step would be to find the associated mean-field orbital ϕ by solving the mean-field equation, which we finally have to write down, for the system in the source $J_0 \circ \hat{\rho}_I$. We obtain the equation by varying ϕ in Eq. (17) and using Eq. (15). Since $\bar{x}$ in the latter is itself a functional of ϕ, the result is complicated:

$$\begin{aligned} &-\frac{\phi''(x)}{2mc_N} - \left[(N-1)g|\phi(x)|^2 - J_0^{\bar{x}}(x) + \frac{(x-\bar{x})}{c_N}\int J_0^{\bar{x}\prime}(y)|\phi(y)|^2dy\right]\phi(x) \\ &+\frac{\mu}{2N}\left[J_0^{\bar{x}\prime\prime}(x) - (x-\bar{x})\int J_0^{\bar{x}\prime\prime\prime}(y)|\phi(y)|^2dy + \frac{(x-\bar{x})^2}{\mu}\int J_0^{\bar{x}\prime\prime}(y)|\phi(y)|^2dy\right]\phi(x) = \ \epsilon\phi(x) \ , \end{aligned} \tag{20}$$

where $J_0^{\bar{x}}(x) \equiv J_0(\frac{x-\bar{x}}{c_N})$ and we have been (and will continue to be) cavalier about factors of c_N in terms of $\mathcal{O}(1/N)$, since they make a difference only in terms of $\mathcal{O}(1/N^2)$, which we have dropped. They could be included in a more accurate functional. We have also added $\bar{x}$'s in the fourth and sixth terms to keep translational invariance manifest; they would otherwise be absorbed into ϵ.

Next, one would need an approximation in which to evaluate/define $\mathcal{E}_1$. As mentioned above, Ref. [12] demonstrates that in the absence of a source the largest corrections to the mean-field approximation in a $1/N$ expansion come from summing ring diagrams. The same statement does not apply to the intrinsic density functional at all possible densities, but the ring sum, which is the leading correction to the mean-field in a "loop-expansion" [15] of $\mathcal{E}[J]$, should yield the $1/N$ corrections near the ground-state intrinsic density and makes a natural choice for $\mathcal{E}_1$.

To obtain an expression for the ring sum, we work with the one-body density matrix ρ_{ab} [16]. We can use it, for starters, to represent the contents of Eq. (20). The left-hand side of that equation, with a delta function $\delta(x-x')$ replacing $\phi(x)$, gives the coordinate-space representation of the mean field $h(x,x')[J_0]$. We can write this h (with spin now included) in an arbitrary space+spin basis in terms of ρ_{ab} :

$$\begin{aligned} h_{ab}[J_0] &= \frac{\partial \mathcal{E}_0[J_0]}{\partial \rho_{ba}} \\ &= \cdots + (J_0^{\bar{x}})_{ab} - \frac{1}{c_N N}\mathrm{Tr}[(J_0^{\bar{x}})'\rho]\,(x-\bar{x})_{ab} \\ &\quad + \frac{1}{2N^2}\left(\mu N (J_0^{\bar{x}})''_{ab} - \mu \mathrm{Tr}[(J_0^{\bar{x}})'''\rho]\,(x-\bar{x})_{ab} + \mathrm{Tr}[(J_0^{\bar{x}})''\rho]\;[(x-\bar{x})^2]_{ab}\right) \ , \end{aligned} \tag{21}$$

where Tr represents a trace over matrix elements, and we have only omitted the terms that do not depend on J_0 in the second and third lines. Hartree-Fock theory corresponds to finding the basis that make h diagonal. Again, we have inserted two $\bar{x}$'s to manifest translational invariance; they just add a constant to all eigenvalues, without altering the Hartree-Fock basis.

The ring sum, in these terms, is just the RPA correlation energy calculated with the effective two-body interaction [16]

$$V_{ab,cd} = \frac{\partial h_{ac}[J_0]}{\partial \rho_{db}} = \frac{\partial^2 \mathcal{E}[J_0]}{\partial \rho_{ca}\partial \rho_{db}} \quad . \tag{22}$$

In coordinate space, this interaction takes the form

$$\begin{aligned} &V(x_1,x_2) = -\frac{g}{c_N}\delta(x_1-x_2) + \frac{1}{2mN}\hat{\mathrm{p}}_1\hat{\mathrm{p}}_2 \\ &-\frac{1}{N}\left[(x_1-\bar{x})\;J_0'(x_2-\bar{x}) + (x_2-\bar{x})\;J_0'(x_1-\bar{x}) - (x_1-\bar{x})(x_2-\bar{x})\left(\int J_0''(y-\bar{x})|\phi^2(y)|dy\right)\right] \\ &+\frac{1}{N^2}[\cdots] \ , \end{aligned} \tag{23}$$

where the term with $\hat{\mathrm{p}}_i \equiv -id/dx_i$ is the two-body center-of-mass Hamiltonian, matrix elments of that term alone are to be antisymmetrized, and we have replaced some more complicated terms with an ellipsis. The extra $\bar{x}$'s we added to h (and to Eq. (23)) have no effect because the particle-hole RPA involves only terms h_{ac} with $a \neq c$ in Eq. (22) and $\bar{x}$ is just a number, with no off-diagonal matrix elements.

The sum of all the ring diagrams can be expressed as [17, 18]

$$E_1[\rho_I] = \mathcal{E}_1[J_0] = \frac{1}{2\pi}\int_0^\infty \mathrm{Re}\left(\mathrm{Tr}\left[\ln(1-\hat{R}(i\omega)\hat{V}) + \hat{R}(i\omega)\hat{V}\right]\right)\,d\omega \quad , \tag{24}$$

where the coordinate-space matrix elements of $\hat{R}(\omega)$ make up the "unperturbed" response function $R(x_1, x_2; x_1', x_2'; \omega)$ for the system in the J_0-dependent mean field. (The spin indices, which we've omitted, just contribute factors of N in Eq. (24).) For zero-range interactions and our source we need these matrix elements only at $x_1 = x_2 \equiv x$, $x_1' = x_2' \equiv x'$, and there the response can be written (for ϕ real) as:

$$R(x, x'; \omega) = \phi(x)\phi(x') \left[\langle x | \frac{1}{\omega + \epsilon + i\eta - \hat{h}[J_0]} | x' \rangle + \langle x' | \frac{1}{-\omega + \epsilon + i\eta - \hat{h}[J_0]} | x \rangle \right] . \quad (25)$$

The matrix elements are just single-particle Green's functions for particles in the mean field. Equation (24) is then the RPA correction to the intrinsic density functional.

One advantage of our definition of intrinsic density (for others, see, e.g., Refs. [10, 19]) is that $\mathcal{E}[J]$ is translationally invariant; moving $\phi(x)$ doesn't change it because it doesn't change ρ_I, the quantity to which J couples. As a result, the RPA equations have a zero mode. With the center-of-mass kinetic energy subtracted subtracted from the Hamiltonian, the zero mode contributes nothing to E_1, but that convenience is not an essential part of the treatment. We could actually start with the full Hamiltonian, with no center-of-mass-energy subtraction, and recover the same result for $E_0 + E_1$. The mean-field energy $E_0[\rho_I]$ would be different, but the difference would be made up [16] by the contribution of the RPA zero mode to E_1, the ring sum in Eq. (24). Further corrections might require mixing of mean-fields with different values of $\bar{x}$ to account for center-of-mass motion, but at RPA order a single-mean field with a proper treatment of the zero mode is sufficient, even without the trick of removing the center-of-mass energy from the Hamiltonian.

Despite this nice feature, Eq. (24) is still a complicated implicit representation of $E_1[\rho_I]$. To solve the Kohn-Sham equation, Eq. (19), we need the derivative of this functional. Taking the derivative is the most numerically involved step in the entire process[2]. References [4, 7] suggest using the relation

$$\frac{\delta E_1[\rho_I]}{\delta \rho_I(x)} = \frac{\delta \mathcal{E}_1}{\delta J_0} \circ \frac{\delta J_0}{\delta \rho_I(x)} \quad , \quad (26)$$

In our model the two terms on the right-hand side can be manageably combined, particularly if we're willing to sacrifice the quality of the functional away from the minimum, a step that, as we shall see, has no effect on the Kohn-Sham solution.

To get $\frac{\delta J_0}{\delta \rho_I}$, one can start by writing ϕ in terms of ρ_I and $\bar{x}$ through the perturbative inversion of Eq. (15) (assuming ϕ real):

$$\phi(x) = (c_N N)^{-1/2} \sqrt{\rho_I(\frac{x - \bar{x}}{c_N}) - \frac{\mu}{2N} \rho_I''(\frac{x - \bar{x}}{c_N}) + \mathcal{O}(\frac{1}{N^2})} \, , \quad (27)$$

Then one could solve Eq. (20) in reverse to obtain $J_0 - \epsilon$ in terms of ϕ. (J_0 is needed only up to a constant to evaluate higher-order corrections.) Though Eq. (20) for J_0 is a complicated differo-integral equation, we can simplify it without harm. Near the ground-state value of ρ_I, the source J_0, which is close to $\delta E_1 / \delta \rho_I$ there, is smaller by $\mathcal{O}(1/N)$ than $(N-1)g|\phi|^2$, the J_0-independent part of the mean-field equation. E_1 is already smaller than E_0 by $\mathcal{O}(1/N)$ near the ground state, and the contributions to E_1 of terms in which J_0 is multiplied by

[2] Ref. [20] discusses some of the difficulties in "orbital-dependent functionals" for atomic and condensed-matter physics.

$1/N$ are therefore down from E_0 by $\mathcal{O}(1/N^2)$. At that order we're already missing terms because of the restriction of the relation between ρ_I and ϕ in Eq. (15) to $\mathcal{O}(1/N)$. Thus, in treating E_1 or its derivative we can neglect the entire second line of Eq. (20), (and even the last term on the first line because the ϕ corresponding to the ground state is symmetric) without changing the Kohn-Sham solution at $\mathcal{O}(1/N)$. This converts the differo-integral equation for J_0 into a simple algebraic one, yielding

$$J_0^{\bar{x}}(x) - \epsilon \approx \frac{1}{2m}\frac{\phi''(x)}{\phi(x)} + Ng|\phi(x)|^2 \ . \tag{28}$$

With this result and Eq. (27) it's easy to get $\delta J_0(y)/\delta\rho_I(x)$ through the chain rule; it would vanish for $x \neq y$ with the approximations just mentioned. One could then extract $\delta E_1[\rho_I]/\delta J_0(y)$ by making local variations in in $J_0(y)$ and calculating the changes in $E_1[\rho_I] = \mathcal{E}_1[J_0]$ through Eq. (24). One could simplify that equation as well by neglecting all but the analogs of the first term after the ellipsis in Eq. (21) and the first two lines of the effective interaction, Eq. (22), without affecting the functional near its minimum at next-to-leading order.

That leaves, finally, the Kohn-Sham equation itself. As mentioned already, one can solve it iteratively. For our intrinsic-density functional that means starting with a guess for J_0, solving the mean-field Eq. (20) to obtain ϕ and ϵ, evaluating E_1 via Eq. (24) and then $\delta E_1/\delta\rho_I(x)$ as just discussed, resetting J_0 to equal $\delta E_1/\delta\rho_I$, and repeating until J_0, E_1, and ϕ (and therefore ρ_I) converge. This is equivalent to solving the mean-field equation (20) with J_0 replaced by $\delta E_1/\delta\rho_I$. And again, because even the leading order terms in E_1 are down by $\mathcal{O}(1/N)$ from E_0 near the minimum, we can throw away the higher-order terms in that equation without affecting the relevant part of E_1. We can even neglect them in constructing $E_0[J_0[\rho_I]]$ near the ground state, because in that functional corrections to the mean-field energy, Eq. (14), are *second* order in the small source J_0. One can get the entire density functional correct at next-to-leading order near the minimum with a Kohn-Sham equation that takes simple Hartree form!

For real nuclei, in which there is more than one spatial orbit, there are no analogs of Eqs. (27) and (28) and our procedure for evaluating $\delta J_0/\delta\rho_I$ won't work. That quantity is the inverse of a generalized linear response function for ρ_I at $\omega = 0$, and will not usually vanish at $y \neq x$, as it did in our machinations above. It be evaluated numerically, but at a high computational cost. Subleading terms can still be neglected in this inverse response function, however, if the only goal is to include the leading corrections to the mean-field functional near the minimum. That would mean ignoring the difference between $\delta J_0/\delta\rho_I(x)$ in Eq. (26) and the ordinary RPA inverse response function, which for a given J_0 can be calculated in a relatively straightforward way [21]. Though $\delta\mathcal{E}_1/\delta J_0$, the other quantity in Eq. (26), might still not easy, it could be evaluated as already described or (particularly for real and more complicated functionals) via the relations in Ref. [20].

If one wanted to avoid even that difficulty, one could make still more approximations without changing the solution. One could even go so far as to evaluate $\delta E_1/\delta J_0$ and $\delta J_0/\delta\rho_I$ at $J_0 = 0$, i.e. at $\rho_I = \langle\hat{\rho}_I(x)\rangle_{\rm mf} = (mgN^2/4)\cosh^{-2}(Nmgx/2)$ (the mean-field approximation to the exact value). That would actually remove J_0 from the right hand side of Eq. (26), thus changing the self-consistent procedure represented by Eq. (19) into a one-step formula:

$$J_0(x) = \int \frac{\delta J_0(y)}{\delta\rho_I(x))}\Big|_{J_0=0} \times \frac{\delta\mathcal{E}_1}{\delta J_0(y)}\Big|_{J_0=0} dy \ , \tag{29}$$

which, after multiplying both sides by the response function $\delta\rho_I(z)/\delta J_0(x)$ (which equals $\delta\rho_I(x)/\delta J_0(z)$), and integrating over x, implies

$$\begin{aligned}\rho_I(x) &= \langle\hat{\rho}_I(x)\rangle_{\rm mf}\big|_{J_0=0} + \int \frac{\delta\rho_I(x)}{\delta J_0(y)}\Big|_{J_0=0} J_0(y)dy + \cdots \\ &= \left[\langle\hat{\rho}_I(x)\rangle_{\rm mf} + \frac{\delta\mathcal{E}_1}{\delta J_0(x)}\right]\Big|_{J_0=0} + \cdots \ . \end{aligned} \tag{30}$$

(The manipulations serve to obtain the second line from the first, which is just a Taylor expansion.) Evaluating Eq. (30) would just be equivalent to calculating the correction to the mean-field ground-state intrinsic density by summing rings generated by the attractive delta function and the first-order insertion of an effective one-body potential (the third term in Eq. (20)) or two-body interaction (the second line of Eq. (22)), with $J(y)$ replaced by $\delta(x-y)$ in both cases because of the functional derivative. That is eminently doable and would reproduce the second line of Eq. (10), the expression for the exact ground-state intrinsic density.

In our model, however, no matter where in this chain of approximations we decided to stop, the intrinsic-density functional would not be local, i.e., it would not look like a Skyrme functional. For that, one would seem to need some form of LDA. The answer to the question at the end of the introduction, then, is that we can write the intrinsic density functional in terms of orbitals, but it's tough, in this model anyway, to make it Skyrme-like. Nonetheless, the successive approximations do bring an important point to light: what we really care about is not so much the density functional for arbitrarily stressed nuclei as it is the ground-state energy and intrinsic density itself. In fact, since the nucleus is never subject to a deforming potential, except in nuclear matter where wave functions are translationally invariant, one might argue that that is *all* we care about. It actually seems a bit strange to apply density-functional theory, the main feature of which is "universality", to a problem in which there are no external influences to treat universally (though density functionals do arise naturally without the accompanying potentials in the density-matrix expansion [3]). In any event, a functional that does not exactly match the definition, Eq. (4) but does give the correct energy and intrinsic density when minimized, and has the additional benefit of being simple, is all we really want for the study of finite nuclei. In the next section we show that in our model, a simple Skyrme-like functional satisfies these requirements.

IV. PHENOMENOLOGICAL FUNCTIONAL AND SKYRME INTERACTIONS

We want a Skyrme-like intrinsic-density functional with a minimum at the correct value to next-to-leading order in $1/N$, that is, a functional that at its minimum reproduces the $\mathcal{O}(N^3)$ and $\mathcal{O}(N^2)$ terms (the latter of which is zero) in Eq. (9), and the second line of Eq. (10) when ρ_I is calculated via Eq. (15). We will reproduce the intrinsic density if the ϕ that solves the Kohn-Sham equation is

$$\begin{aligned}\phi(x) &\equiv \phi_0(x) + \frac{1}{N}\phi_1(x) \\ \phi_0(x) &= \frac{\sqrt{(N-1)mg}}{2}\left[\cosh^{-1}(\frac{Nmgx}{2c_N})\right] \\ \phi_1(x) &= s\frac{\sqrt{(N-1)mg}}{4}\left[\frac{3}{2}\cosh^{-3}(\frac{Nmgx}{2c_N}) - \cosh^{-1}(\frac{Nmgx}{2c_N})\right] \ , \end{aligned} \tag{31}$$

where $s \equiv 1 + m^2 g^2 N^2 \mu_{\rm gs}/2 = 1 + \pi^2/6$, and the c_N's appear because of their presence in Eq. (15).

To express such a functional through the formalism detailed above, we need to keep the center-of-mass kinetic energy in the Hamiltonian and use an effective nucleon mass

$$m^* = \frac{m}{1+\alpha/N} \ , \tag{32}$$

where α is a constant to be determined later[3]. We denote by $E_0^*[\rho_I]$ the mean-field functional obtained by changing $E_0[\rho_I]$ in Eq. (18) in that way (both changes affect the kinetic term), and write the functional through first order in $1/N$ as

$$E[\rho_I] = E_0^*[\rho_I] + E_1[\rho_I] \ , \qquad E_1[\rho_I] = -\int dx \left(\frac{\beta g}{2N} \rho_I^2 + \frac{\gamma}{6m^* N^3} \rho_I^3 \right) \ , \tag{33}$$

where β and γ are also constants to be determined later. Eq. (19), with the omission of all but the first three terms in Eq. (20) (which we argued could be neglected without changing the minimum of the functional), leads to the explicit Kohn-Sham-like equation

$$-\frac{\phi''}{2m^*} - (N-1+\beta) g |\phi|^2 \phi - \frac{\gamma}{2m^* N} |\phi|^4 \phi = \epsilon \phi \ . \tag{34}$$

Inserting $\phi = \phi_0 + \phi_1/N$ into this equation, writing $\epsilon \equiv \epsilon_0 + \epsilon_1/N$, and expanding in inverse powers of $(N-1)$ rather than N (because of the c_N's in Eq. (31)), we find at leading order in $(N-1)^{-1}$ the self-consistent equation

$$-\frac{1}{2m}\phi_0'' - (N-1) g |\phi_0|^2 \phi_0 = \epsilon_0 \phi_0 \ . \tag{35}$$

At $\mathcal{O}(1/[N-1]) \equiv \mathcal{O}(1/N)$, assuming ϕ real, we have

$$-\frac{1}{2m}\phi_1'' - 3(N-1) g \phi_0^2 \phi_1 - \frac{\alpha}{2m}\phi_0'' - (N-1) g \beta \phi_0^3 - \frac{\gamma}{2m}\phi_0^5 = \epsilon_0 \phi_1 + \epsilon_1 \phi_0 \tag{36}$$

Now, the solution to Eq. (35) is the ϕ_0 of Eq. (31), with $\epsilon_0 = -mg^2(N-1)^2/8$. The solution to Eq. (36), with the appropriate ϕ_0 and ϵ_0 plugged in, is the ϕ_1 of Eq. (31), provided $\beta = \alpha - 2s$, $\gamma = 18s$, and $\epsilon_1 = \alpha \epsilon_0$. The requirement that the energy $E[\rho_I]$ in Eq. (33) have no $\mathcal{O}(N^2)$ term at the minimum is satisfied as well if and only if

$$\alpha = 2(1 + \frac{4s}{5}) \ , \quad \beta = 2(1 - \frac{s}{5}) \ , \quad \gamma = 18s \ . \tag{37}$$

Thus, minimizing our functional in Eq. (33) with these values of the parameters yields the correct energy and intrinsic density to $\mathcal{O}(1/N)$.

The functional can be extended to reproduce ρ_I and E at higher orders in $(1/N)$ with the addition of higher powers of ρ_I/N^2, though finding the corresponding coefficients gets harder. These functionals, as discussed, do not converge to the "exact one" for all ρ_I, but they do around the ground-state ρ_I. The result suggests that real Skyrme functionals, which

[3] Though an effective mass can be included through the use of an intrinsic kinetic-energy density [22], we will simply alter the nucleon mass here.

may be viewed as depending on intrinsic semilocal kinetic, spin-orbit, and current densities in addition to the ordinary intrinsic density, behave the same way; we have no reason to think them correct away from the minimum.

It's worth noting that the construction above is even more straightforward if we take $\rho_I(x) \equiv N|\phi(x+\bar{x})|^2$ rather than define it as the expectation value of $\hat{\rho}_I$ in the the Slater determinant constructed from ϕ, i.e., as in Eq. (15). We do the latter only because the mean-field approximation and, more importantly, *real Skyrme functionals* work better with that definition [14]. The success of the wave-function-based assignment $\rho_I \equiv \langle \hat{\rho}_I \rangle_{\rm mf}$ raises the hope that Skyrme functionals can be derived and improved through mean-field theory with some effective low-momentum interaction, with the addition of relatively small corrections. The density-matrix expansion works along those lines, and deserves more attention. It remains to be seen whether the formalism presented here — the inversion method modified for self-bound systems — can be happily married to such an approach.

We have said nothing here about "symmetry restoration", a technique that, particularly in its rotational form, is viewed as a step beyond the local or semi-local Skyrme-mean-field equations. The projected-mean-field equations, while more complicated than their unprojected counterparts, are still equations for single-particle orbitals, however. Symmetry-restored mean-field theory is simply a more accurate starting point for the inversion method than plain mean-field theory. Presumably, additional corrections can be absorbed into those equations, as they were here. This statement, of course, says nothing about what the corrected functionals will look like.

To summarize, we have shown that a version of the Hohenberg-Kohn theorem holds for the intrinsic density in self-bound system and that, to the extent that a convergent expansion around mean-field solutions exists for such systems, a Kohn-Sham-like procedure can be applied to obtain functionals of the intrinsic density that include all correlations. Skyrme functionals seem to be approximations to the exact intrinsic-density functionals but it is quite possible that, like our phenomenological functional, they work poorly away from the ground-state density and energy. On the other hand, we do not always need them to do more than that, and a concerted effort to improve even this limited kind of functional is worthwhile. The density-matrix expansion, which can clearly be applied more accurately than it was 35 years ago, may offer improvements and should be further explored.

Fruitful discussions with A. Bhattacharyya, T. Duguet, R.J. Furnstahl, T. Schaefer, and A. Schwenk are gratefully acknowledged. This work was supported in part by the U.S. Department of Energy under Contract DE-FG02-97ER41019.

---

[1] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).
[2] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
[3] J. W. Negele, Phys. Rev. C **1**, 1260 (1970).
[4] M. Valiev and G. W. Fernando (1997), cond-mat/9702247.
[5] R. Fukuda, T. Kotani, Y. Suzuki, and S. Yokojima, Prog. Theor. Phys. **92**, 833 (1994).
[6] S. Weinberg, *The Quantum Theory of Fields, Vol.2: Modern Applications* (Cambridge University Press, 1996).
[7] S. J. Puglia, A. Bhattacharyya, and R. J. Furnstahl, Nucl. Phys. A **723**, 145 (2002).
[8] K. Okamura, Int. J. Mod. Phys. **11**, 65 (1996).
[9] J. B. McGuire, J. Math. Phys. **5**, 622 (1964).

[10] F. Calogero and A. Degasperis, Phys. Rev. A **11**, 265 (1975).
[11] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. C **62**, 054311 (2000).
[12] B. Yoon and J. W. Negele, Phys. Rev. A **16**, 1451 (1977).
[13] K. W. Schmid and P.-G. Reinhard, Nucl. Phys. A **530**, 283 (1991).
[14] P.-G. Reinhard and J. Engel (2006), in preparation.
[15] J. W. Negele and H. Orland, *Quantum Many-Particle Systems* (Westview Press, 1988).
[16] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer-Verlag, New York, 1980).
[17] J. P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems* (The MIT Press, 1986).
[18] Y. R. Shimizu, P. Donati, and R. A. Broglia, Phys. Rev. Lett. **85**, 2260 (2000).
[19] D. V. Neck and M. Waroquier, Phys. Rev. C **58**, 3359 (1998).
[20] E. Engel, *in A Primer in Density Functional Theory* (C. Fiolhais, F. Nogueira, and M. Marques, eds., Springer, 1997).
[21] S. Shlomo and G. F. Bertsch, Nucl. Phys. A **243**, 507 (1975).
[22] A. Bhattacharyya and R. J. Furnstahl, Nucl. Phys. A **747**, 268 (2005).